1135-65-1574 **Chao Yang***, 1 Cyclotron Rd, Berkeley, CA 94720. *Solving Large-scale Eigenvalue Problems in Electronic Structure Calculations.*

One of the most time consuming tasks in Kohn-Sham density functional based electronic structure calculations is to compute eigenpairs of a Hermitian matrix. The number of eigenpairs to be computed is proportional to the number of atoms in the poly-atomic systems being studied. For large molecules and nanoclusters, this number can be quite large even though it is still a small fraction of the dimension of the matrix. For these problems, many standard iterative methods that use the Rayleigh-Ritz procedure to extract approximate eigenpairs from a single subspace becomes very costly. We examine a number of techniques to overcome this difficulty and improve the efficiency and scalability of the eigenvalue calculation on large-scale high performance parallel computers. (Received September 23, 2017)